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Transport and Fate of Selected Organic Pollutants in a Sandy Soil

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Chloroform,1,2-dibromo-3-chloropropane, dichlorobromomethane, 1,2-dichloroethane, tetrachloroethene, 1,1,2-trichloroethane, trichloroethene, chlorobenzene, toluene, nitrobenzene, and bis(2-chloroethyl)ether percolated rapidly through the soil; retardation factors were 2.5 or less. Less mobility was exhibited by 1,4-dichlorobenzene and 1,2,4-trichlorobenzene, with retardation factors of 3.4 and 9.4, respectively. Significant losses due to volitilization and/or degradation were observed in some cases, but were not usually sufficient to prevent transport of appreciable quantities of pollutants through the lengths of the columns.

A simple mathematical model based on water solubility of the compound and the organic C content of the soil predicted the retardation factors of the pollutants within a factor of three.

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Transport and Fate of Selected Organic Pollutants in a Sandy Soil[1]

J. T. WILSON, C. G. ENFIELD, W. J. DUNLAP, R. L. COSBY, D. A. FOSTER, AND L. B. BASKIN[2]

ABSTRACT

Ground waters are increasingly vulnerable to pollution by organic chemicals that migrate through the soil mantle. To assess the minimal protection that soil can be expected to provide ground water, the transport and fates of 13 organic pollutants were studied in a sandy soil with low organic matter content (0.087% organic C). Glass columns were packed with soil to a depth of 140 cm in a manner that preserved to the maximum extent possible the characteristics of the original soil profile. In separate experiments, the columns received 14 cm/day of water containing a mixture of approximately 1.0 or 0.2 mg/liter of each of the organic compounds. Quantities of compounds that volatilize from the soil surface were measured, as well as concentrations in the column effluent.

Chloroform (trichloromethane), 1,2-dibromo-3-chloropropane, dichlorobromomethane, 1,2-dichloroethane, tetrachloroethene, 1,1,2-trichloroethane, and trichloroethene were not degraded in this soil. These compounds percolated rapidly through the soil; their retardation factors (velocity of tritiated water through soil divided by apparent velocity of pollutant through soil) were 2.5 or less. Between 19 and 65% of the material applied to the surface percolated to a depth of 140 cm, and the remainder volatilized.

Chlorobenzene, 1,4-dichlorobenzene, and 1,2,4-trichlorobenzene also percolated through the soil; retardation factors were 1.7, 3.4, and 9.4, respectively. Between 26 and 49% of the material applied reached 140 cm.

Toluene and nitrobenzene degraded in some of the columns but not in others. In the absence of degradation, 60 and 80% of nitrobenzene and 13% of toluene applied to the soil surface reached 140 cm. The retardation factors were 2.3 or less.

Bis(2-chloroethyl)ether did not degrade; 86% of the material applied reached 140 cm, and the compound's retardation factor was <1.5.

A simple mathematical model based on water solubility of the compound and the organic C content of the soil predicted the retardation factors of the pollutants within a factor of three.

Additional Index Words: chloroform, dichlorobromomethane, 1,2-dichloroethane, tetrachloroethene, 1,1,2-trichloroethane, trichloroethene, chlorobenzene, 1,4-dichlorobenzene, 1,2,4-trichlorobenzene, toluene, nitrobenzene, bis(2-chloroethyl)ether, tetrachloroethylene, trichloroethylene, 1,2-dibromo-3-chloropropane.

Wilson, J. T., C. G. Enfield, W. J. Dunlap, R. L. Cosby, D. A. Foster, and L. B. Baskin. 1981. Transport and fate of selected organic pollutants in a sandy soil. J. Environ. Qual. 10:501-506.

The number and quantity of organic chemicals produced in the United States has increased steadily during the last four decades, resulting in the current production of more than 40,000 compounds. The manufacture, transport, use, and disposal of these chemicals are resulting in the release of significant quantities of many organic substances into soil, where they are subject to possible transport into underlying ground water by recharge water infiltrating through the unsaturated zone. Many of these compounds are toxic or potentially toxic. Nevertheless, for many years this problem has been largely ignored and essentially undefined, principally because of an inflated concept of the capacity of the soil to attenuate pollution from organic substances, and because of the difficulties inherent in the analysis of trace organic chemicals.

Recently, however, growing concern for groundwater quality coupled with the availability of vastly improved analytical methodology for organic compounds have resulted in increased monitoring of ground water for organic pollutants. This work is revealing widespread pollution of ground water by organic chemicals, clearly indicating significant movement of many of these substances through the soil. Some specific examples are: occurrences of trichloroethene in many ground waters in both the United States and Europe as the result of spills, leaks, and soil disposal of wastes (Giger et al., 1978; Zoeteman et al., 1980; Buller, 1979; Weimar, 1980); occurrence of 1,2-dibromo-3-chloropropane (DBCP) in ground water in areas in California where it was applied to soils as a nematocide (Peoples et al., 1980); pollution of a large body of ground water by phenol in the vicinity of an accidental spill of this compound in Wisconsin (Baker et al., 1978); and, the movement into ground water of 4,4′-methylene bis(2-chloroaniline) from a waste-water lagoon in Michigan (Parris et al., 1980).

Clearly, preservation of the quality of our valuable and irreplaceable ground-water resources requires prudent control of the release of organic chemicals into the soil. To establish control measures that will adequately protect ground water and yet permit reasonable utilization of the subsurface as a waste receptor, definitive information concerning the behavior of organic chemicals in subsurface environments must be developed. This investigation was designed to develop quantitative information concerning the fate and transport of selected organic pollutants in an unsaturated soil. Emphasis was placed on halogenated compounds of low molecular weight, many of which are indicated by the monitoring data cited above to be serious pollutants of ground water.

METHODS AND MATERIALS

Soil from the Lincoln fine sand, a mixed, thermic Typic Ustifluvent, was collected in 10-cm increments from a profile near Ada, Okla. (see Table 1). Columns of borosilicate glass process pipe, 5 cm i.d by 150 cm (Ace Glass Inc., Vineland, N.J.) were packed with the soil to a depth of 140 cm. Each 10-cm increment was packed in the same relative position it occupied in the original soil. The average bulk density of the columns was 1.65 g/cm³.

The saturated hydraulic conductivity of the packed columns ranged from 120 to 190 cm/day. The columns received 14 cm of water per day, which resulted in unsaturated flow through almost the entire length of the columns. To protect the biota, the soil was not dried or sieved, and the columns were packed soon after collection of the soil. To minimize problems of sorption of applied compounds or leaching of contaminants from the column and associated plumbing, all ma-

[1]Contribution of the Robert S. Kerr Environmental Research Laboratory, U.S. Environmental Protection Agency, Ada, Okla. Received 11 July 1980.

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pgs. 501-506

Table 1—Characterization of soil samples.

Soil properties	Column study Average	Column study Range†	Field site Average	Field site Range†
pH	6.4	6.6 - 6.1	ND‡	
CEC	3.5	4.8 - 2.3	ND	
		%		
Sand	92	95 -89	76	91 -64
Silt	5.9	8.0 - 4.0	5.7	9.4 - 3.0
Clay	2.1	3.5 - 1.5	19	33 - 2.6
Organic-C	0.087	0.22- 0.02	0.13	0.25- 0.05

† From 1 to 150 cm.
‡ Not determined.

terials contacting the feed solution, soil, and column effluent were made of either borosilicate glass or Teflon.

The experimental configuration is presented in Fig. 1. To minimize loss of compounds by volatilization, the feed solution was stored inside a Teflon gas-sampling bag with a Teflon septum valve (Alltech Assoc., Arlington Heights, Ill.). The bag was fitted inside a sealed glass container filled with water. Water was pumped into the container around the bag with a peristaltic metering pump, which forced the feed solution from the bag onto the soil column.

Breathing quality air was delivered to the headspace above the soil at a pressure of 2 cm of water. Approximately 12 ml/min of air was removed from the headspace; this produced an air exchange about once every 8 min. The bottom of the column had a single port cap that was packed with Pyrex glass wool. Effluent from the column was collected in a Teflon gas-sampling bag fitted with a Teflon plug valve. The bag was immersed in 5 cm of water to prevent air from the headspace from passing through the soil and inflating the bag. The Teflon bags had minimal headspace and effectively contained the volatile compounds in both the feed and the sample. The feed solution was kept on ice, while the columns were maintained at 20 ± 1°C. The feed solution was replaced daily.

The columns were dosed with spring water having the following characteristics: pH = 7.2; HCO_3^- alkalinity = 513 ppm; Ca^{2+} = 76 ppm; Mg^{2+} = 35 ppm; Na^+ = 52 ppm; Cl^- = 5 ppm; SO_4^{2-} = 17 ppm; NO_3^- + NO_2^--N = 1 ppm; NH_4^+-N <0.05 ppm; and o-PO_4^{3-}-P = 0.01 ppm. One column in each experiment received spring water alone and served as an analytical control. Three replicate columns received spring water amended with the organic compounds. A mixture of the organic compounds was added to water and stirred until visible turbidity disappeared. Headspace in the container was kept to a minimum and the container was sealed to prevent loss of the more volatile compounds. Actual concentrations in the water applied to the soil were monitored (Table 2). In the first experiment the water was dosed with approximately 1 mg/liter of the compounds listed in Table 2. The feed solution also was dosed with 1 mg/liter of 2-chlorophenol, 2,4-dichlorophenol, 2,4,6-trichlorophenol, 4-nitrophenol, diethylphthalate, and bis(2-ethylhexyl)phthalate; these compounds will not be discussed due to difficulties in analysis or to great variability in their measured concentrations in the feed solution. In the second experiment, the compounds listed in Table 2 were added at a concentration of 0.2 mg/liter, except for trichlorobenzene, which was added at a concentration of 5 mg/liter.

The feed solution was applied for 45 days (20 pore-water volumes); all compounds reached steady-state concentrations in the column effluent after 25 days. Estimates of material that volatilized or remained in the column effluent are averages of quantities determined on at least 4 sampling days for each of the three columns after that compound reached steady state in the column effluent. The volume of pore water in each column was determined from the retention volume of tritiated water. The retardation factor for a compound was calculated as the number of retention volumes eluted when the concentration of that compound was one-half the concentration in the feed solution.

Analytical Procedures

Concentrations of chloroform, 1,2-dichloroethane, dichlorobromomethane, 1,1,2-trichloroethane, 1,2-dibromo-3-chloropropane, tetrachloroethene, toluene, and chlorobenzene were determined by procedures proposed by EPA (1979b), based on the method of Bellar and Lichtenberg (1974). A 25-ml sample of feed solution or column effluent was transferred to a modified purger on a Tekmar LSC-2 Liquid Sample Concentrator (Tekmar Corp., Cincinnati, Ohio). Volatile compounds were purged from solution with He and collected in a trap (28 cm by 1.8 mm i.d.) packed with Tenax resin. Purging efficiency ranged from 49 to 98%. The trap was then heated and the compounds that desorbed were determined by gas chromotography using a flame ionization detector. The same traps were used to collect volatiles from the headspace of the soil columns. A trap was placed on each column for 1.0 hour, then the sorbed compounds were determined as described above.

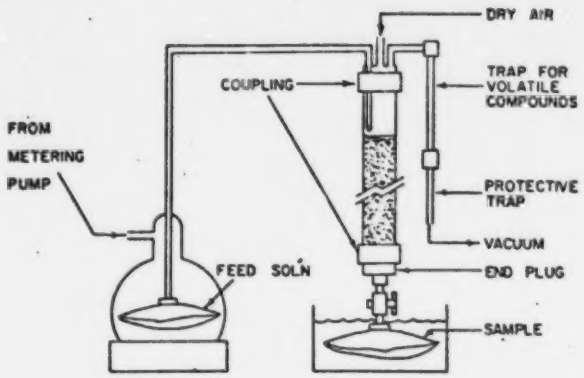

Fig. 1—Experimental apparatus.

Solution concentrations of chlorobenzene, 1,4-dichlorobenzene, 1,2,4-trichlorobenzene, nitrobenzene, and bis(2-chloroethyl)ether were determined after extraction into methylene chloride. A 200-ml sample was extracted successively with 35, 25, and 25 ml of solvent. The combined extracts were dried with anhydrous Na_2SO_4, then concentrated to 0.5 ml by Kuderna-Danish and micro-Snyder distillation. Extraction efficiencies ranged from 58 to 74%. Each sample of column effluent was collected for roughly 20 hours; the volume of sample, about 300 ml, represented approximately one-half the pore water volume of the columns.

Sand, silt, and clay content were determined by sedimentation according to procedure D422-54T prescribed by ASTM (1958).

Total organic carbon (TOC) in soil was determined by combustion with a Leco WR-12 Carbon Analyzer (Leco Corp., St. Joseph, Mo.). Crushed soil (1.0 g) was stripped of inorganic C by immersion in 15% HCl for 4 hours. The soil was dried overnight at 120°C and then analyzed.

Cation exchange capacity (CEC) of soil was determined by Na saturation (Chapman, 1965). Alkalinity, forms of N, and PO_4 in water samples were determined according to procedures prescribed by EPA (1979a). Calcium and magnesium were determined with a Jarrel-Ash inductively coupled argon-plasma emission spectrograph (Fischer Scientific, Waltham, Mass.) according to procedures recommended by EPA (1979c).

RESULTS AND DISCUSSION

Fate

A mass balance for 12 of the compounds was calculated after the concentration of the compound in the column effluent reached a steady state, that is, after the apparent sorptive capacity of the soil for the compound had been saturated. Data are presented in Table 2 for two initial concentrations of each compound.

For dichlorobromomethane and tetrachloroethene, apparently more material was recovered than was applied to the soil. The quantity applied and the quanti-

Table 2—Fate of organic compounds applied to a sandy soil.

Compound	Concentration applied	Volatilized	Column effluent	Degraded or not accounted for
	mg/liter	% of material applied		
Halogenated hydrocarbons:				
Chloroform	0.90	54 ± 9†	41 ± 4†	5 ± 11†
	0.25	61 ± 10	31 ± 9	8 ± 14
Dichlorobromomethane	0.82	54 ± 14	48 ± 4	− 2 ± 17
	0.18	94 ± 16	45 ± 17	−39 ± 18
1,2-Dichloroethane	0.81	49 ± 9	61 ± 9	−10 ± 14
	0.25	50 ± 7	37 ± 5	+13 ± 11
Tetrachloroethene	0.15	101 ± 29	19 ± 16	−20 ± 7
1,1,2-Trichloroethane	1.00	27 ± 16	65 ± 12	8 ± 10
	0.16	47 ± 13	61 ± 5	− 8 ± 7
Trichloroethene	0.90	58 ± 14	28 ± 1	14 ± 15
	0.18	88 ± 18	21 ± 13	− 9 ± 11
Substituted benzenes:				
Chlorobenzene	1.04	27 ± 7	33 ± 9 (23 ± 4)‡	40 ± 7 (50 ± 10)‡
	0.18	54 ± 21	26 ± 15 (34 ± 24)	20 ± 21 (12 ± 13)
1,4-Dichlorobenzene	0.80	ND§	37 ± 4	63 ± 4
	0.13	ND	49 ± 10	51 ± 10
1,2,4-Trichlorobenzene	3.40	ND	46 ± 11	54 ± 32
	0.57	ND	39 ± 3	61 ± 20
Toluene	0.90	38 ± 11	2 ± 1.7	60 ± 8
	0.20	66 ± 19	13 ± 6	21 ± 15
Nitrobenzene	0.92	ND	80 ± 29	20 ± 25
	0.16	ND	60 ± 20	40 ± 31
Miscellaneous:				
Bis(2-chloroethyl)ether	0.86	ND	91 ± 15	9 ± 31
	0.16	ND	86 ± 1	14 ± 20

† Means ± 95% confidence intervals.
‡ Material in effluent as determined by the purge and trap method.
§ Not determined.

ty in the column effluent were determined by the same method and would share any systematic bias. It is likely that the quantity volatilized was overestimated, which reduced the sensitivity of the experiment to degradation. However, if extensive degradation had occurred (e.g. >50% of the material applied), it would have been detected for at least one concentration of each compound. There was no evidence of extensive degradation of the halogenated hydrocarbons. This is not surprising because these compounds are generally recalcitrant to biodegradation (McConnell et al., 1975).

Despite their volatility, significant portions of all the compounds percolated through the soil. To evaluate the influence of soil on the volatilization of halogenated aliphatic hydrocarbons, the experimentally measured flux of five compounds volatilizing from the soil surface was compared to the flux expected from free water (Table 3). The expected flux from free water was calculated from half-lives for volatilization (Dilling, 1977) experimentally determined at concentrations and temperature near those encountered in this study.

$$\text{Flux from water} = 0.693\ VC/t_{1/2},$$

where

$t_{1/2}$ = volatilization half-life in Dilling's system,
V = ml of water under 1.0 cm² in Dilling's system, and
C = μg of compound/ml of column effluent in this study.

Table 3—Flux of volatile organic compounds from soil and water.

Compound	Concn. applied	Measured from soil	Calculated from water
	mg/liter	μg/cm² per hour	
Chloroform	0.9	0.38	3.9
1,2-Dichloroethane	0.81	0.38	4.8
1,1,2-Trichloroethane	1.00	0.36	5.0
Trichloroethene	0.90	0.34	3.0
Tetrachloroethene	0.15	0.103	1.8

The concentration of organic compound in the column effluent, rather than that in the feed, was used in the calculations to provide a conservative estimate of the flux from the water. The average flux from soil was calculated as follows:

$$\text{Flux from soil} = DAF/S,$$

where

D = μg compound/ml of feed solution,
A = ml of feed solution applied/hour,
F = fraction of material applied that volatilized (Table 2), and
S = surface area of column (cm²).

Compared to volatilization from water, the soil inhibited volatilization by an order of magnitude (Table 3). The results are similar to those of Kilzer et al. (1979), who found that volatilization from a sandy soil was inhibited by roughly an order of magnitude for seven of the 10 compounds they investigated. Many of the compounds in this study volatilized at similar rates (Table 3); this would not be surprising if the flux of volatiles from the soil was limited by diffusion through the air-filled pores because the compounds have similar molecular weights and Henry's law constants (Dilling, 1977).

Significant proportions of the substituted benzenes also percolated through the soil (Table 2). Although all the substituted benzenes examined in this study are biodegradable to some extent (Alexander and Lustigman, 1966; Malaney and McKinney, 1966; Marinucci and Bartha, 1979), the soil biota did not prevent migration of these compounds through the soil (Table 2).

Toluene is easily degraded in sewage (Malaney and McKinney, 1966) and seawater (Walker and Colwell, 1976), and is degraded by a variety of soil microorganisms (Kaplan and Hartenstein, 1979). In this study, toluene was degraded when applied at 0.9 mg/liter, but not at 0.2 mg/liter (Table 2). However, when a second sample of soil was dosed with 0.2 mg/liter toluene and 5 mg/liter 1,2,4-trichlorobenzene, >60% of the toluene originally applied was degraded (data not shown). The failure of toluene to degrade (Table 2) when degradation should be expected illustrates the need for caution when extrapolating laboratory studies to the field. Biodegradation studies only indicate a potential for degradation, which may or may not be realized in the field at a particular place and time.

Nitrobenzene is extensively and rapidly degraded in adapted activated sludge (Pitter, 1976). However, degradation of nitrobenzene by soil microorganisms can be slow, with more than 64 days required for complete

disappearance (Alexander and Lustigman, 1966). In this study, nitrobenzene was extensively degraded in one of the three columns when applied at 0.92 mg/liter (Fig. 2). This degradation appeared abruptly 3 weeks after the beginning of the experiment. The occurrence has not been explained—it could represent a lag period required for the active microbial population to reach the necessary density to affect the concentration of nitrobenzene, reflect a mutation allowing an organism to metabolize the compound under conditions where it previously could not, or be caused by a shift in the microbial community that favored nitrobenzene-degrading organisms.

Chlorobenzene can be metabolized by benzene-acclimated activated sludge (Malaney and McKinney, 1966) and by phenol-acclimated sludge (Chambers et al., 1963). In this study, chlorobenzene applied at 0.18 mg/liter did not degrade, while a major fraction of chlorobenzene applied at 1.04 mg/liter was unaccounted for. This could represent biodegradation at the higher concentration.

Trichlorobenzenes can be degraded in soil, although very slowly (Marinucci and Bartha, 1979). Using the kinetic coefficients determined by Marinucci and Bartha (1979) for a relatively fertile soil, and assuming Michaelis-Menten kinetics, biodegradation would have destroyed only 0.3% of the 1,2,4-trichlorobenzene applied in this study. The 1,2,4-trichlorobenzene that was unaccounted for in this study probably volatilized or was subject to some other abiotic process.

Transport

The halogenated aliphatic hydrocarbons, toluene, nitrobenzene, and bis(2-chloroethyl)ether, moved readily through Lincoln fine sand (Table 4); in no case was the retardation factor >2.5. Retardation of chlorinated benzenes generally increased with decreasing water solubility. Chlorobenzene was reasonably mobile

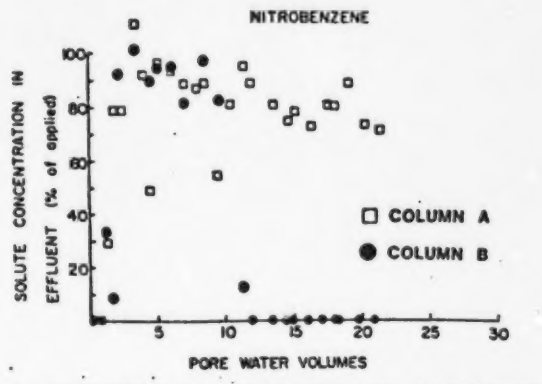

Fig. 2—Biodegradation and lack of biodegradation of nitrobenzene in replicate soil columns at 0.9 mg/liter.

while 1,2,4-trichlorobenzene was significantly retained by the soil.

Transport of many compounds through soil is retarded with respect to water due to sorption to soil solids. Sorption of certain pesticides and other relatively complex organic compounds applied to soil frequently follows the Freundlich adsorption equation, that is, $S = KC^n$, where C is the concentration in solution (mg/liter), S is the quantity sorbed (μg/g soil), and K and n are constants (Hâmaker and Thompson, 1972; Rao and Davidson, 1979). When n is significantly different from 1, the concentration of the organic compound influences the rate of migration of the compound through soil; when n is near 1, the equation reduces to a simple linear sorption isotherm, $S = KC$, and the concentration of the compound has little influence on the rate of its migration (Rao and Davidson, 1979).

Unfortunately, good data on loadings and solution concentrations of organic pollutants in actual field situ-

Table 4—Retention of organic compounds by soils.

Compound	Molecular weight	Water solubility	Retardation factor†			Predicted retardation factor
			Field	Columns		
				Experiment 1	Experiment 2	
		mg/liter				
Halogenated hydrocarbons:						
Chloroform	119	8,000‡		<1.5	<1.5	1.2
1,2-Dibromo-3-chloropropane	236	1,230§		Not done	2.1 ± 0.5#	1.8
Dichlorobromomethane	164	No data		<1.5	<1.5	Not done
1,2-Dichloroethane	99	8,690‡		<1.5	<1.5	1.2
Tetrachloroethene	166	150‡		Not done	2.5 ± 0.2	3.2
1,1,2-Trichloroethane	133	4,500‡		<1.5	<1.5	1.2
Trichloroethene	132	1,100‡		1.6 ± 0.2	1.5 ± 0.2	1.6
60 cm			>2.4, 1.6			2.0
150 cm			3.1, 2.3			1.7
Substituted benzenes:						
Chlorobenzene	113	500‡		1.7 ± 0.2	4.9 ± 0.5	1.9
1,4-Dichlorobenzene	147	79‡		3.4 ± 0.3	3.7 ± 0.4	4.0
1,2,4-Trichlorobenzene	181	28.6¶		9.4 ± 0.3	8.0 ± 0.2	7.0
Toluene	92	515‡		<2	<2	1.8
Nitrobenzene	123	1,900‡		2.3 ± 0.5	1.5 ± 0.2	1.4
Miscellaneous:						
Bis(2-chloroethyl)ether	143	10,200‡		<1.5	<1.5	1.2

† Interstital water velocity/velocity of pollutant.
‡ Verschueren (1977).
§ Chiou et al. (1979).
¶ This study.
# 95% confidence interval.

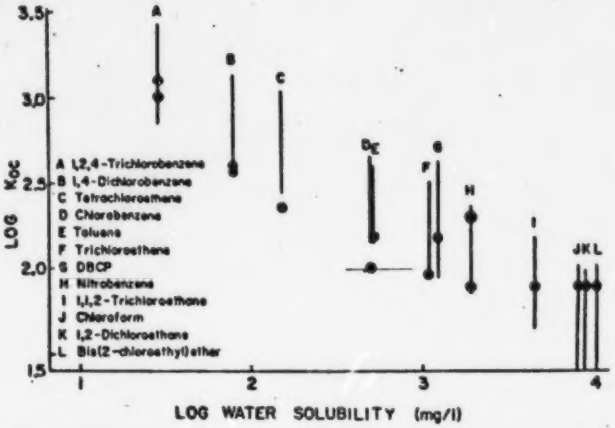

Fig. 3—Relationship between the water solubility of a compound (mg/liter) and its partition coefficient between soil organic C and soil solution (K_{oc}).

ations such as spills or leaking dump sites are rarely available, partly because need for the information occurs after the fact, often many years after. As a result, accurate description of the movement of organic pollutants through soils and subsurface materials will likely be restricted to those compounds that follow linear sorption isotherms. Fortunately, many compounds of environmental interest do exhibit linear sorption isotherms; examples include several halogenated aliphatic hydrocarbons (Chiou et al., 1979), polynuclear aromatic hydrocarbons (Means et al., 1980), dibenzothiophene (Hassett et al., 1980), and benzene (Rogers, 1980).

Assuming singular equilibrium adsorption-desorption models and a linear adsorption isotherm, the retardation of the compound with respect to water is:

$$R = 1 + (\varrho/\theta)K = V/V_p \text{ (Hashimoto et al., 1964)}, \quad [1]$$

where

ϱ = bulk density of the soil (g/cm³),
θ = volumetric water content (ml/cm³),
K = soil solids to soil solution distribution coefficient (ml/g),
V = intersitial pore water velocity (Darcy velocity/θ), and
V_p = apparent velocity of pollutant through soil.

If the organic-C content of the soil is known, K can be predicted from the soil organic-C to water partition coefficient (K_{oc}) of a compound:

$$K = (K_{oc})\text{ (g organic C/g dry soil)}. \quad [2]$$

Several researchers have estimated the K_{oc} of a compound from its water solubility:

$$\log G = 4.04 - 0.557 \log WS_1$$

(Chiou et al., 1979), [3]

$$\log K_{oc} = -0.54 \log WS_2 + 0.44$$

(Karickhoff et al., 1979), and [4]

$$\log K_{oc} = 3.64 - 0.55 \log WS_3$$

(Kenega, 1980); [5]

where

WS_1 = water solubility (μmol/liter),
WS_2 = water solubility (mole fraction),
WS_3 = water solubility (mg/liter), and
G = partition coefficient based on organic matter ($K_{oc} = G/1.724$).

These empirical relationships were developed using batch sorption studies. Figure 3 compares the K_{oc} data from this study (solid circles) with the range of the three estimates of K_{oc} presented above (lines). In general, the agreement is acceptable, even though relationships developed for equilibrium batch experiments are being applied to a dynamic system.

The predicted retardation factor was calculated from Eq. [1], [2], and [3] based on a weighted-average organic C content for the soil column. The equation of Chiou et al. (1979) was used because their regression equation was calculated from the properties of many of the same compounds examined in this study. There is good agreement between the predicted retardation factor and the experimental data (Table 4). The only serious disparity is chlorobenzene in the second experiment, where actual retardation was significantly greater than predicted. This may reflect a significant nonlinearity in the sorption isotherm of chlorobenzene to soil solids. However, in the second experiment, chlorobenzene was added in the presence of a 25-fold greater concentration of 1,2,4-trichlorobenzene. It is also possible that sorption of trichlorobenzene to soil organic matter increased the capacity of the organic matter to sorb chlorobenzene. In any case, this observation emphasizes the need to consider potential interactions among pollutants that may influence the behavior of complex mixtures of organic wastes.

At the end of experiment 2, the compounds in the feed solution were replaced with 10 mg/liter 1,2-dibromo-3-chloropropane (DBCP) and the transport of this compound monitored. As predicted by the model, DBCP was very mobile in this soil (Table 4). A mass balance for DBCP could not be calculated, due to a failure in the analytical procedure for the quantity of DBCP that volatilized. However, the concentration of DBCP in the column effluent reached the original concentration in the feed solution, indicating little volatilization or degradation.

Field Studies

The results of the column studies and of the mathematical model were verified for trichloroethene in an in situ soil profile (Table 1). The soil is a Konawa fine sandy loam, a thermic, Ultic Haplustalf. The site had previously been instrumented to measure hydraulic conductivity; selected tensiometers were converted to suction lysimeters for sampling. A purger from the Liquid

Sample Concentrator was taken to the field and connected to a suction lysimeter. Soil water was pulled through the lysimeter into the purger with a peristaltic pump. Then the volatile compounds were purged from solution with N_2 (40 ml/min for 15 min) and collected on a trap, which was returned to the laboratory for analysis. The procedure and sampling site has been described in detail elsewhere (Wood et al., 1981).

Chloride was used as a tracer for the movement of water. The retardation factor for trichloroethene was calculated as the ratio of the time required for trichloroethene and the Cl^- to reach a particular sampler at a particular depth. Although the agreement was not as close as in the column study, the model provided a reasonably accurate estimate of the mobility of trichloroethene in an in situ soil profile (Table 4).

CONCLUSIONS

Most of the organic pollutants examined in this study were transported readily through soil, which explains the increasingly frequent occurrence of these compounds in ground water. Ground waters underlying soils with low organic matter content are vulnerable to pollution by chloroform, 1-2-dibromo-3-chloropropane, dichlorobromomethane, 1,2-dichloroethane, tetrachloroethene, 1,1,2-trichloroethane, trichloroethene, toluene, nitrobenzene, and bis(2-chloroethyl) ether, and to a lesser extent by chlorobenzene, 1,2-dichlorobenzene and 1,2,4-trichlorobenzene.

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